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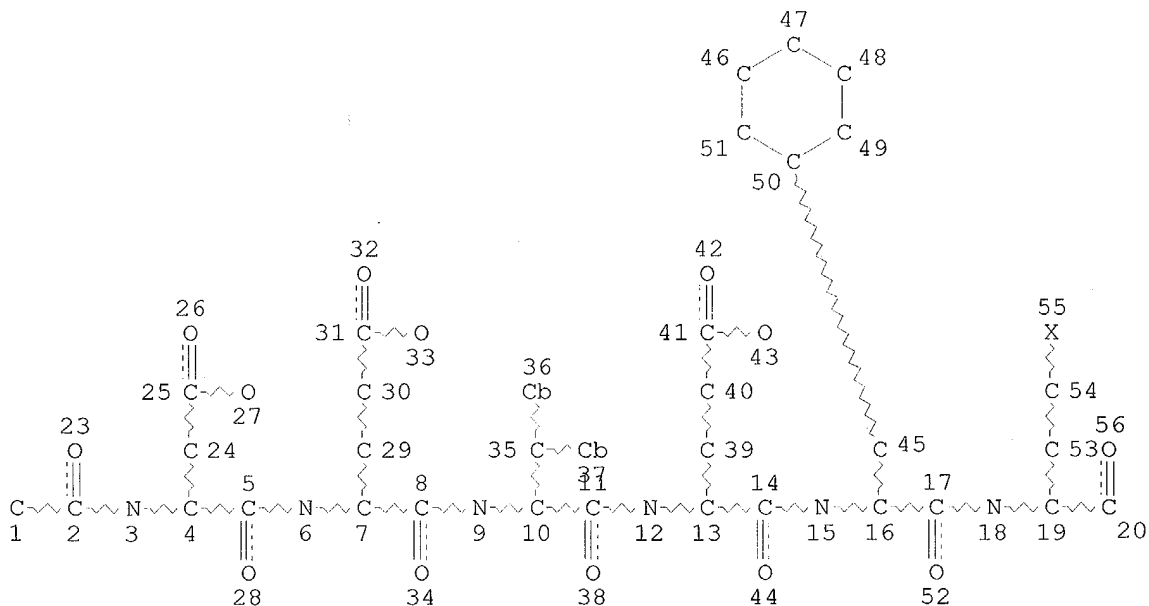
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FILE COVERS 1907 - 29 Sep 2003 VOL 139 ISS 14  
 FILE LAST UPDATED: 28 Sep 2003 (20030928/ED)

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 L3 STR



NODE ATTRIBUTES:  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:  
 RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 54

STEREO ATTRIBUTES: NONE

L5 23 SEA FILE=REGISTRY SSS FUL L3  
L6 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L5

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=> d ibib abs hitrn l6 1-6

L6 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN  
ACCESSION NUMBER: 2002:777963 HCAPLUS  
DOCUMENT NUMBER: 137:295254  
TITLE: Preparation of peptide inhibitors of hepatitis C virus  
NS3 protease  
INVENTOR(S): Colarusso, Stefania; Gardelli, Cristina; Gerlach, Benjamin; Harper, Steven; Koch, Uwe; Matassa, Victor Giulio; Muraglia, Ester; Narjes, Frank; Ontoria, Ontoria Jesus Maria; Petrocchi, Alessia; Ponzi, Simona; Stansfield, Ian; Summa, Vincenzo  
PATENT ASSIGNEE(S): Istituto di Ricerche di Biologia Molecolare P. Angeletti Spa, Italy; et al.  
SOURCE: PCT Int. Appl., 151 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002079234	A1	20021010	WO 2002-EP3435	20020326
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.: GB 2001-7924 A 20010329  
OTHER SOURCE(S): MARPAT 137:295254  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Compds. I, II, and III [X = CH<sub>2</sub>, O; Y = CRa<sub>2</sub>, where Ra = H, OH, CO<sub>2</sub>H, alkyl, (hetero)aryl, (hetero)aralkyl, or CRa<sub>2</sub> = cycloalkyl; Z = (un)substituted (hetero)aryl; R<sub>2</sub> = alkyl, fluoroalkyl, or CH<sub>2</sub>SH; R<sub>3</sub> = (un)substituted alkyl, (hetero)aryl, (hetero)aralkyl, or together with NRC forms a ring; R<sub>c</sub> = H or alkyl or NRC together with R<sub>3</sub> forms a ring; R<sub>4</sub> = alkyl, alkenyl, (hetero)aralkyl, (hetero)aryl or an acidic group; R<sub>5</sub> = (un)substituted carbamoyl, acyl, carboxylic ester, oxalyl, or sulfonyl group, which may be attached to an amino acid or a di- or tripeptide; R<sub>13</sub> is a group contg. .ltoreq. 25 carbon atoms, 0-5 oxygen atoms, 0-3 nitrogen atoms, 0-2 sulfur atoms and .ltoreq. 9 other heteroatoms which may be the same or different; R<sub>17</sub> is H, alkyl, alkenyl, (hetero)aryl, (hetero)aralkyl, OH, alkoxy, aryloxy, (hetero)aralkoxy, thioether, sulfonyl or sulfoxide group; R<sub>18</sub> is a group contg. .ltoreq. 25 carbon atoms, 0-5 oxygen atoms, 0-3 nitrogen atoms, 0-2 sulfur atoms and .ltoreq.

9 other heteroatoms which may be the same or different] and their pharmaceutically-acceptable salts or esters were prepd. as inhibitors of the hepatitis C virus (HCV) NS3 protease. Thus, i-BuO<sub>2</sub>C-Glu-Leu-Cys-NHCH<sub>2</sub>CH<sub>2</sub>C<sub>6</sub>H<sub>3</sub>Cl<sub>2</sub>-2,4 was prepd. by the solid-phase method and showed IC<sub>50</sub> .ltoreq. 10 .mu.M for inhibition of NS3 protease.

IT 467440-27-3P 467440-28-4P 467440-45-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptide inhibitors of hepatitis C virus NS3 protease)

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:116982 HCAPLUS

DOCUMENT NUMBER: 137:47425

TITLE: Evolution, synthesis and SAR of tripeptide .alpha.-ketoacid inhibitors of the hepatitis C virus NS3/NS4A serine protease

AUTHOR(S): Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Muraglia, Ester; Conte, Immacolata; Stansfield, Ian; Matassa, Victor G.; Narjes, Frank

CORPORATE SOURCE: Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 705-708

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:47425

AB N-Terminal truncation of the hexapeptide ketoacid MeCO-Asp-Glu-NHCH(CHPh<sub>2</sub>)CO-Glu-NHCH(CH<sub>2</sub>c-C<sub>6</sub>H<sub>11</sub>)CONHCH(CH<sub>2</sub>CHF<sub>2</sub>)CO<sub>2</sub>H (all-L stereochem.) (c-C<sub>6</sub>H<sub>11</sub>= cyclohexyl) gave rise to potent tripeptide inhibitors of the hepatitis C virus NS3 protease/NS4A cofactor complex. Optimization of these tripeptides led to ketoacid BOC-NHCH(c-C<sub>5</sub>H<sub>9</sub>)CO-Leu-NHCH(CH<sub>2</sub>CHF<sub>2</sub>)COCO<sub>2</sub>H (all-L stereochem.) (BOC = tert-butoxycarbonyl, c-C<sub>5</sub>H<sub>9</sub> = cyclopentyl) with an IC<sub>50</sub> of 0.38 .mu.M. The SAR of these tripeptides is discussed in the light of the recently published crystal structures of a ternary tripeptide/NS3/NS4A complexes.

IT 262437-54-7

RL: PAC (Pharmacological activity); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent)  
(prepn. and structure-activity relationship of tripeptide ketoacid inhibitors of hepatitis C virus serine protease)

IT 262437-54-7DP, derivs.

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(prepn. and structure-activity relationship of tripeptide ketoacid inhibitors of hepatitis C virus serine protease)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:116981 HCAPLUS

DOCUMENT NUMBER: 137:149812

TITLE: A designed P1 cysteine mimetic for covalent and

AUTHOR(S): Narjes, Frank; Koehler, Konrad F.; Köch, Uwe; Gerlach, Benjamin; Colarusso, Stefania; Steinkuhler, Christian; Brunetti, Mirko; Altamura, Sergio; De Francesco, Raffaele; Matassa, Victor G.

CORPORATE SOURCE: Department of Chemistry, MRL Rome, IRBM, Rome,

SOURCE: Pomezia, 00040, Italy  
Bioorganic & Medicinal Chemistry Letters (2002),  
12(4), 701-704  
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The difluoromethyl group was designed by computational chem. methods as a mimetic of the canonical P1 cysteine thiol for inhibitors of the hepatitis C virus NS3 protease. This modification led to the development of competitive, non-covalent inhibitor AcAspGlu-NHCH(CHPH2)CO-Glu-NHCH(CH2C6H11)CONHCH(CH2CHF2)R (I, R = CHO) Ki 30 nM and reversible covalent inhibitors (I, R = CO2H) Ki 0.5 nM; and (I, R = COCO2H) Ki\* 10 pM.

IT 252355-84-3 252355-85-4 252355-86-5  
262437-54-7 444990-66-3 444990-67-4  
444990-68-5 444990-69-6 444990-70-9

RL: PAC (Pharmacological activity); BIOL (Biological study)  
(designed P1 cysteine mimetic for covalent and non-covalent inhibitors of HCV NS3 protease)

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2000:352482 HCAPLUS

DOCUMENT NUMBER: 133:189820

TITLE: Probing the active site of the hepatitis C virus serine protease by fluorescence resonance energy transfer

AUTHOR(S): Fattori, Daniela; Urbani, Andrea; Brunetti, Mirko; Ingenito, Raffaele; Pessi, Antonello; Prendergast, Kristine; Narjes, Frank; Matassa, Victor G.; De Francesco, Raffaele; Steinkuhler, Christian

CORPORATE SOURCE: Istituto di Ricerche di Biologia Molecolare "P. Angeletti", Rome, 00040, Italy

SOURCE: Journal of Biological Chemistry (2000), 275(20), 15106-15113  
CODEN: JBCHA3; ISSN: 0021-9258

PUBLISHER: American Society for Biochemistry and Molecular Biology

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A serine protease domain contained within the viral NS3 protein is a key player in the maturational processing of the hepatitis C virus polyprotein and a prime target for the development of antiviral drugs. In the present work, we describe a dansylated hexapeptide inhibitor of this enzyme. Active site occupancy by this compd. could be monitored following fluorescence resonance energy transfer between the dansyl fluorophore and protein tryptophan residues and could be used to (1) unambiguously assess active site binding of NS3 protease inhibitors, (2) directly det. equil. and pre-steady-state parameters of enzyme-inhibitor complex formation, and (3) dissect, using site-directed mutagenesis, the contribution of single residues of NS3 to inhibitor binding in direct binding assays. The assay was also used to characterize the inhibition of the NS3 protease by its cleavage products. We show that enzyme-product inhibitor complex formation depends on the presence of an NS4A cofactor peptide. Equil. and pre-steady-state data support an ordered mechanism of ternary (enzyme-inhibitor-cofactor) complex formation, requiring cofactor complexation prior to inhibitor binding.

IT 262437-54-7

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)  
(inhibitor; probing the active site of the hepatitis C virus NS3 serine

proteinase by fluorescence resonance energy transfer)  
 REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 2000:68910 HCAPLUS  
 DOCUMENT NUMBER: 132:245829  
 TITLE: .alpha.-Ketoacids Are Potent Slow Binding Inhibitors  
 of the Hepatitis C Virus NS3 Protease  
 AUTHOR(S): Narjes, Frank; Brunetti, Mirko; Colarusso, Stefania;  
 Gerlach, Benjamin; Koch, Uwe; Biasiol, Gabriella;  
 Fattori, Daniela; De Francesco, Raffaele; Matassa,  
 Victor G.; Steinkuehler, Christian  
 CORPORATE SOURCE: Departments of Biochemistry Medicinal Chemistry and  
 Computational Chemistry, Istituto di Ricerche di  
 Biologia Molecolare (IRBM) P. Angeletti, Pomezia,  
 00040, Italy  
 SOURCE: Biochemistry (2000), 39(7), 1849-1861  
 CODEN: BICHAW; ISSN: 0006-2960  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The replication of the hepatitis C virus (HCV), an important human  
 pathogen, crucially depends on the proteolytic maturation of a large viral  
 polyprotein precursor. The viral nonstructural protein 3 (NS3) harbors a  
 serine protease domain that plays a pivotal role in this process, being  
 responsible for four out of the five cleavage events that occur in the  
 nonstructural region of the HCV polyprotein. We here show that  
 hexapeptide, tetrapeptide, and tripeptide .alpha.-ketoacids are potent,  
 slow binding inhibitors of this enzyme. Their mechanism of inhibition  
 involves the rapid formation of a noncovalent collision complex in a  
 diffusion-limited, electrostatically driven assocn. reaction followed by a  
 slow isomerization step resulting in a very tight complex. PH dependence  
 expts. point to the protonated catalytic His 57 as an important  
 determinant for formation of the collision complex. Ki values of the  
 collision complexes vary between 3 nM and 18.5 .mu.M and largely depend on  
 contacts made by the peptide moiety of the inhibitors. Site-directed  
 mutagenesis indicates that Lys 136 selectively participates in  
 stabilization of the tight complex but not of the collision complex. A  
 significant solvent isotope effect on the isomerization rate const. is  
 suggestive of a chem. step being rate limiting for tight complex  
 formation. The potency of these compds. is dominated by their slow  
 disocn. rate consts., leading to complex half-lives of 11-48 h and  
 overall Ki values between 10 pM and 67 nM. The rate consts. describing  
 the formation and the disocn. of the tight complex are relatively  
 independent of the peptide moiety and appear to predominantly reflect the  
 intrinsic chem. reactivity of the ketoacid function.

IT 252355-84-3P 262437-54-7P 262437-57-0P  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological  
 study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU  
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES  
 (Uses)

(prepn. of .alpha.-ketoacids as potent slow binding inhibitors of  
 hepatitis C virus NS3 protease)

REFERENCE COUNT: 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2003 ACS on STN  
 ACCESSION NUMBER: 1999:795834 HCAPLUS  
 DOCUMENT NUMBER: 132:36034  
 TITLE: Preparation of peptide inhibitors of hepatitis C virus  
 NS3 protease  
 INVENTOR(S): Matassa, Victor; Narjes, Frank; Koehler, Konrad;

PATENT ASSIGNEE(S): Ontoria, Jesus; Poma, Marco; Marchetti, Antonella  
 Istituto Di Ricerche Di Biologia Molecolare P  
 Angeletti S.p.A., Italy  
 SOURCE: PCT Int. Appl., 121 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9964442	A1	19991216	WO 1999-GB1824	19990609
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2330247	AA	19991216	CA 1999-2330247	19990609
AU 9942798	A1	19991230	AU 1999-42798	19990609
AU 754773	B2	20021121		
EP 1084137	A1	20010321	EP 1999-955475	19990609
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
PRIORITY APPLN. INFO.: GB 1998-12523 A 19980610				
WO 1999-GB1824 W 19990609				

AB Fluorinated oligopeptides Y-B-A-X or Y-B-A'-X' [A is an amino acid residue NHCH(CH<sub>2</sub>CHF<sub>2</sub>)(CH<sub>2</sub>)mCO and A' is NHCHR<sub>1</sub>(CH<sub>2</sub>)mCO (m = 0, 1; R<sub>1</sub> is a fluorine-substituted hydrocarbyl side chain); B is a naturally or non-naturally occurring amino acid residue NHCHR<sub>2</sub>CO (R<sub>2</sub> is a nonpolar or polar but uncharged side chain or is a side chain contg. an acidic functionality); X = CO<sub>2</sub>R<sub>8</sub>, H, OR<sub>8</sub>, CF<sub>3</sub>, CONR<sub>9</sub>R<sub>10</sub>, NHSO<sub>2</sub>R<sub>25</sub>, or certain 5-membered heterocyclic groups (R<sub>8</sub>, R<sub>9</sub>, R<sub>10</sub>, R<sub>25</sub> = H, alkyl, alkenyl, aryl, aralkyl); X' = NHSO<sub>2</sub>N<sub>25</sub>; Y = Z-F-E-D-C (C is a natural or non-natural amino acid residue having non-polar, polar but uncharged, or acidic side chains; D, E, and F may be absent or represent a natural or non-natural amino acid; Z is absent, H, or R<sub>7</sub>CO which forms an amide, urethane, or urea linkage with the nitrogen atom to which it is attached) or R<sub>13</sub>CO (R<sub>13</sub> is an aliph. or arom. group contg. 1-25 carbon atoms, 0-5 oxygen atoms, 0-3 nitrogen atoms, 0-2 sulfur atoms, and up to 9 other heteroatoms)] were prepd. as inhibitors of hepatitis C virus NS3 protease. Thus, Ac-Asp-Glu-Met-Glu-Glu-NHCH(CH<sub>2</sub>CHF<sub>2</sub>)CO<sub>2</sub>H-(S), prepd. by coupling of (S)-tert-Bu 2-amino-4,4-difluorobutanoate hydrochloride with protected pentapeptide, showed IC<sub>50</sub> for inhibition of NS3 protease.

IT 252355-84-3P 252355-85-4P 252355-86-5P  
 252355-87-6P 252355-88-7P 252355-89-8P  
 252355-90-1P 252355-91-2P 252355-93-4P  
 252355-94-5P 252355-95-6P 252355-96-7P  
 252355-97-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of peptide inhibitors of hepatitis C virus NS3 protease)

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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FILE COVERS 1907-1966  
 FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

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STRUCTURE FILE UPDATES: 28 SEP 2003 HIGHEST RN 594810-89-6  
 DICTIONARY FILE UPDATES: 28 SEP 2003 HIGHEST RN 594810-89-6

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

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Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:  
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

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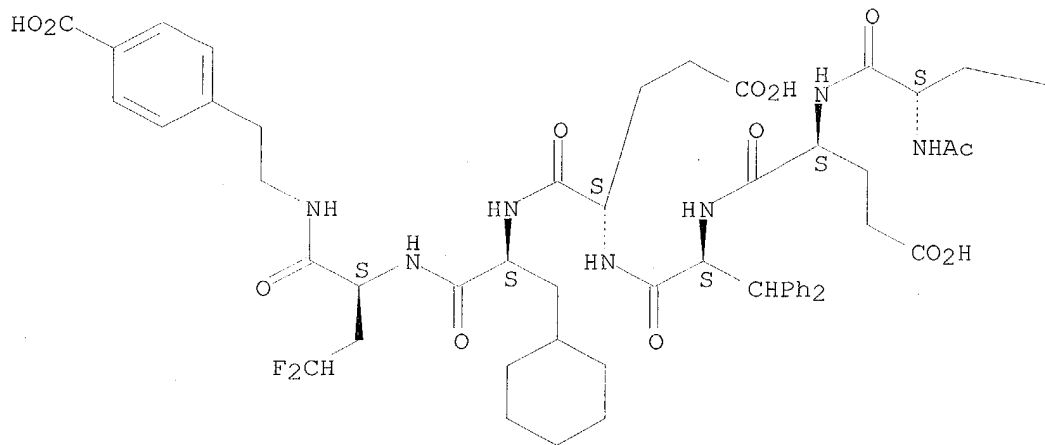
L5 ANSWER 1 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 467440-45-5 REGISTRY  
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 FS PROTEIN SEQUENCE; STEREOSEARCH

MF C53 H65 F2 N7 O15  
 SR CA  
 LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

CO<sub>2</sub>H

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

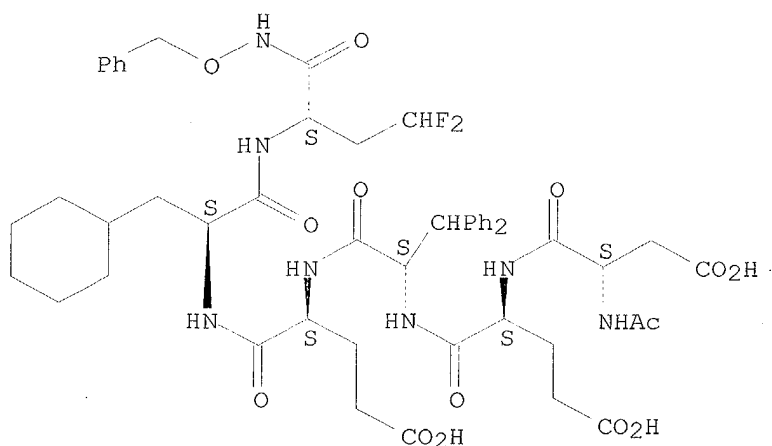
REFERENCE 1: 137:295254

L5 ANSWER 2 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 467440-28-4 REGISTRY  
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 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C51 H63 F2 N7 O14  
 SR CA  
 LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.





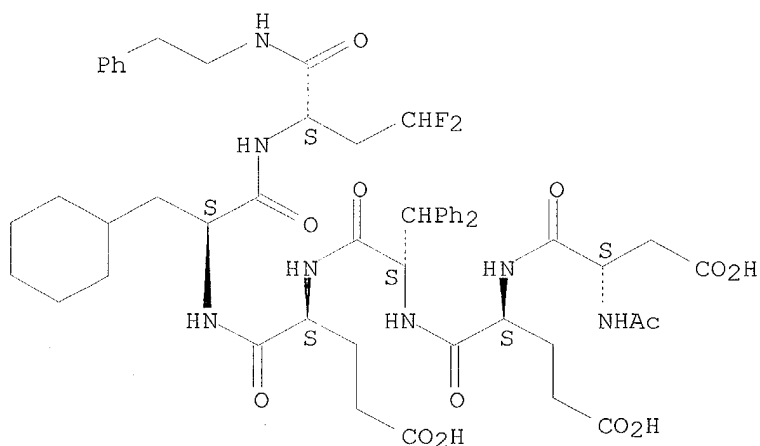
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:295254

L5 ANSWER 3 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 467440-27-3 REGISTRY  
CN Butanamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-L-alanyl-2-amino-4,4-difluoro-N-(2-phenylethyl)-, (2S)- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C52 H65 F2 N7 O13  
SR CA  
LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



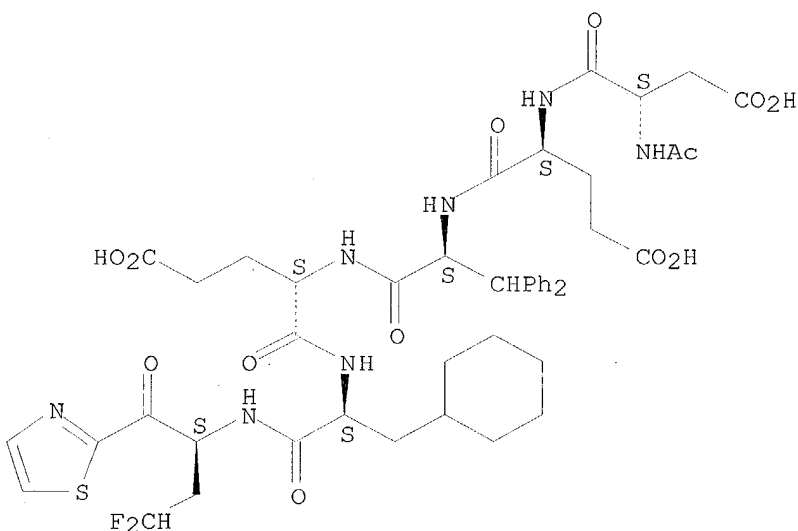
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:295254

L5 ANSWER 4 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 444990-70-9 REGISTRY  
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-  
 phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[(1S)-3,3-difluoro-  
 1-(2-thiazolylcarbonyl)propyl]- (9CI) (CA INDEX NAME)  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C47 H57 F2 N7 O13 S  
 SR CA  
 LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



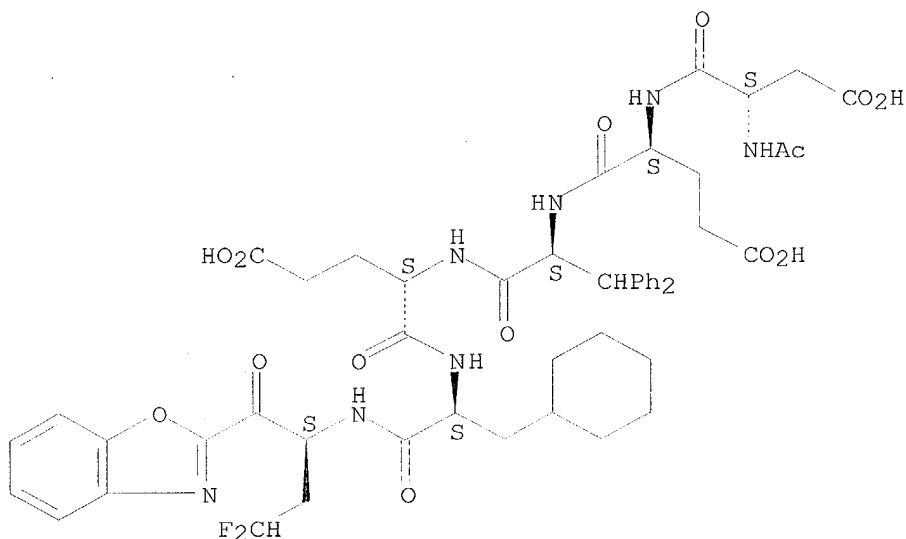
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

L5 ANSWER 5 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 444990-69-6 REGISTRY  
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-  
 phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[(1S)-1-(2-  
 benzoxazolylcarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX  
 NAME)  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C51 H59 F2 N7 O14  
 SR CA  
 LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



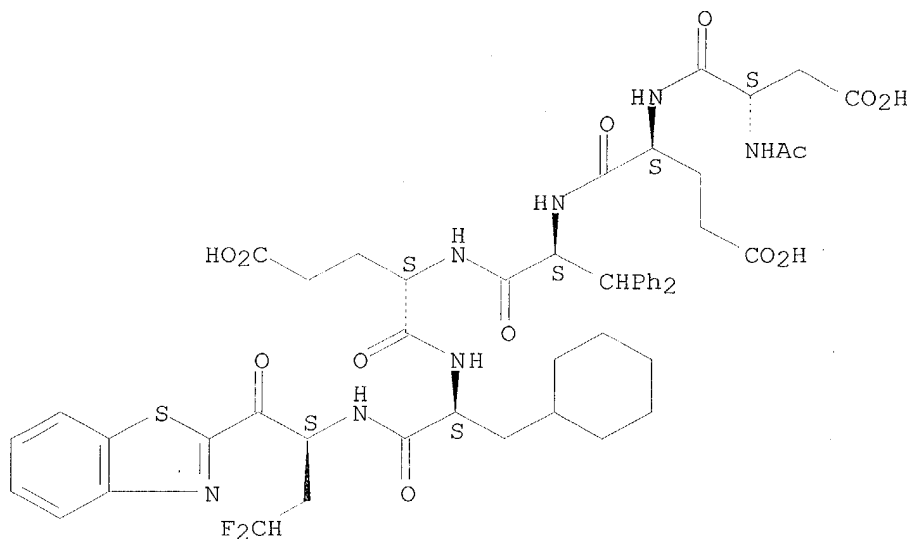
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

L5 ANSWER 6 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 444990-68-5 REGISTRY  
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-  
phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[(1S)-1-(2-  
benzothiazolylcarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX  
NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C51 H59 F2 N7 O13 S  
SR CA  
LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



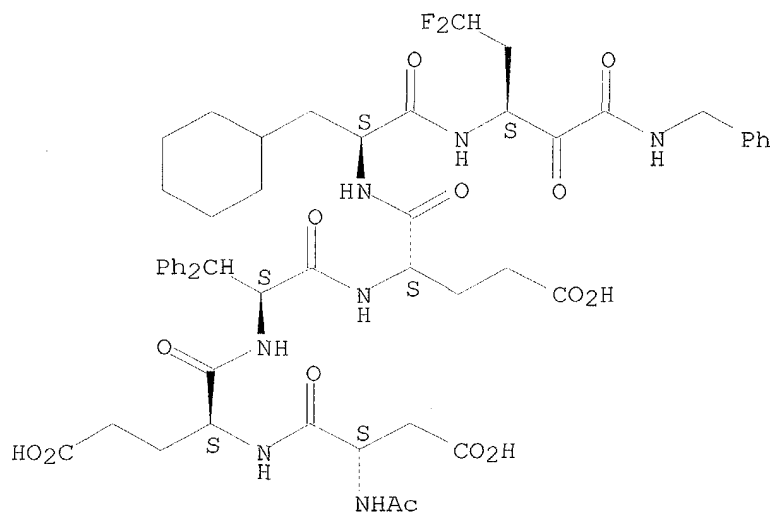
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

L5 ANSWER 7 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 444990-67-4 REGISTRY  
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-  
phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[(1S)-1-(2,2-  
difluoroethyl)-2,3-dioxo-3-[(phenylmethyl)amino]propyl]- (9CI) (CA INDEX  
NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C52 H63 F2 N7 O14  
SR CA  
LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



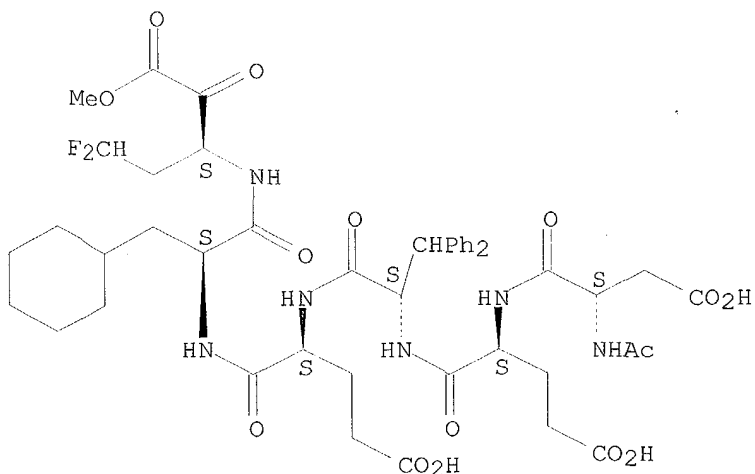
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

L5 ANSWER 8 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 444990-66-3 REGISTRY  
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[(1S)-1-(2,2-difluoroethyl)-3-methoxy-2,3-dioxopropyl]- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C46 H58 F2 N6 O15  
SR CA  
LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

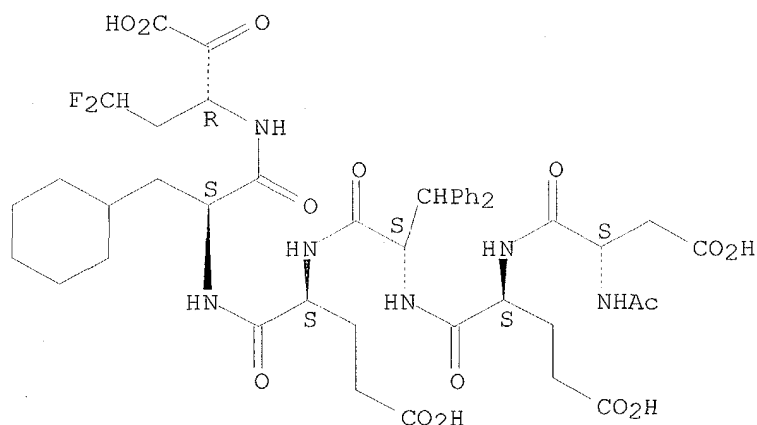
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

L5 ANSWER 9 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 262437-57-0 REGISTRY  
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[(1R)-1-(carboxycarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C45 H56 F2 N6 O15  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



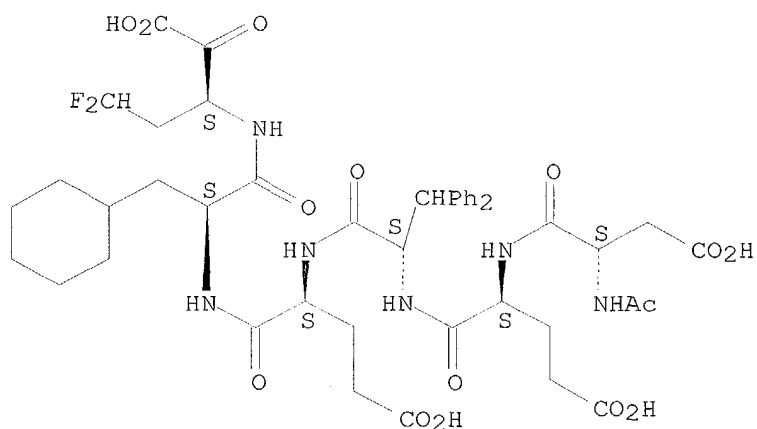
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:245829

L5 ANSWER 10 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 262437-54-7 REGISTRY  
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[(1S)-1-(carboxycarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C45 H56 F2 N6 O15  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



4 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

REFERENCE 2: 137:47425

REFERENCE 3: 133:189820

REFERENCE 4: 132:245829

L5 ANSWER 11 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN

RN 252355-97-8 REGISTRY

CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[3,3-difluoro-1-(2-furanylcarbonyl)propyl]- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

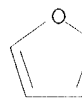
MF C48 H58 F2 N6 O14

SR CA

LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

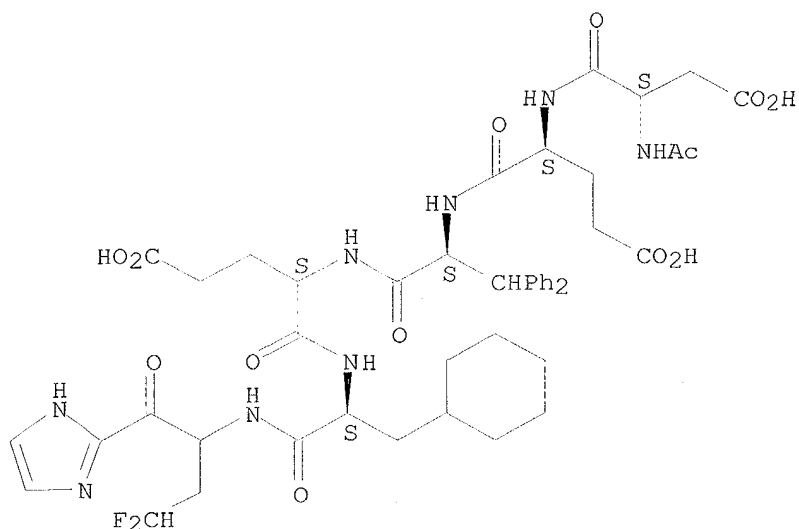
REFERENCE 1: 132:36034

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L5 ANSWER 12 OF 23  REGISTRY  COPYRIGHT 2003 ACS on STN
RN 252355-96-7  REGISTRY
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-
phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[3,3-difluoro-1-
(1H-imidazol-2-ylcarbonyl)propyl]- (9CI)  (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C47 H58 F2 N8 O13
SR CA
LC STN Files:  CA, CAPLUS
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\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.





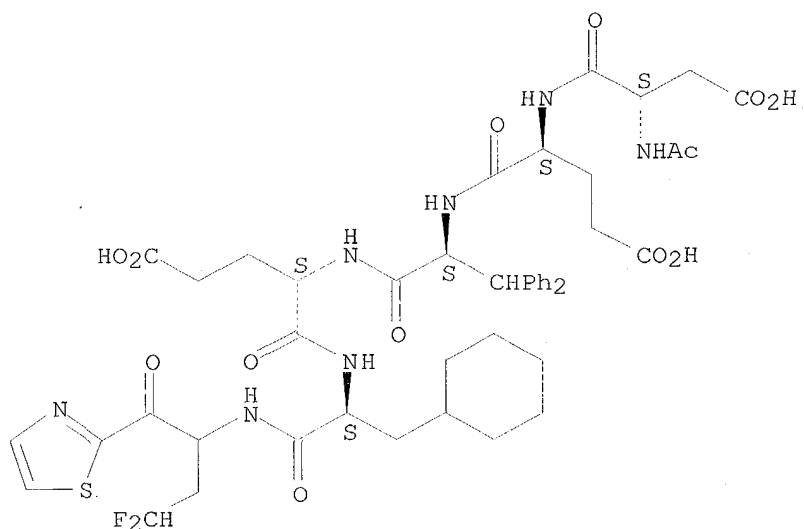
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 13 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 252355-95-6 REGISTRY  
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[3,3-difluoro-1-(2-thiazolylcarbonyl)propyl]- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C47 H57 F2 N7 O13 S  
SR CA  
LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



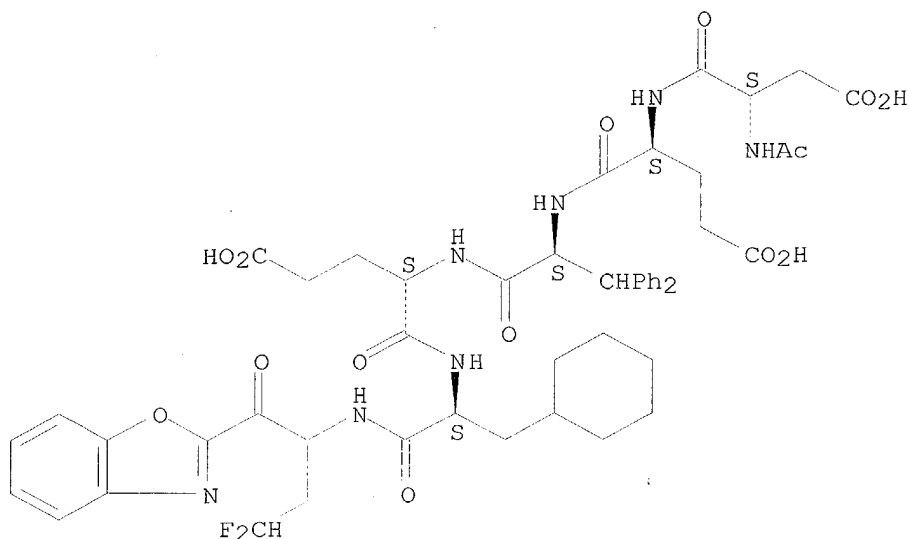
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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 14 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 252355-94-5 REGISTRY  
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[1-(2-benzoxazolylcarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C51 H59 F2 N7 O14  
SR CA  
LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



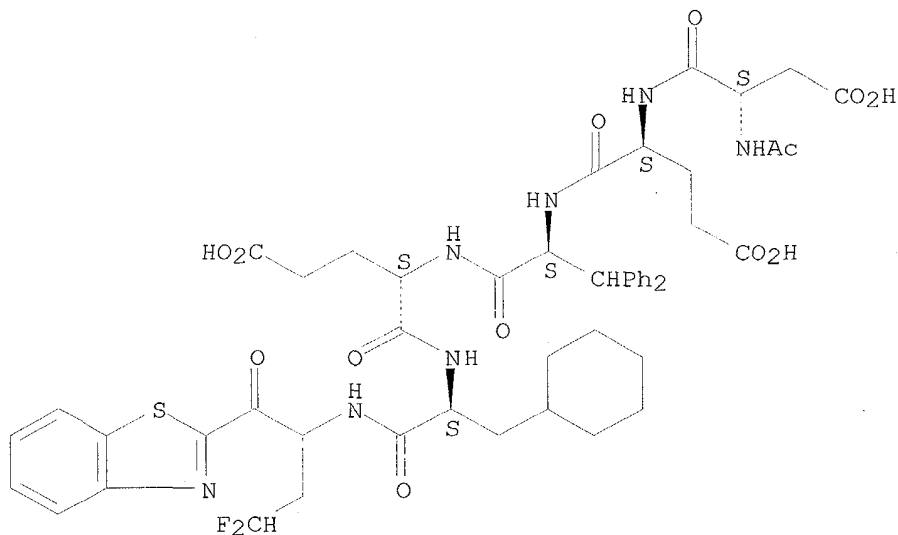
1 REFERENCES IN FILE CA (1907 TO DATE)  
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REFERENCE 1: 132:36034

L5 ANSWER 15 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 252355-93-4 REGISTRY  
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[1-(2-benzothiazolylcarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C51 H59 F2 N7 O13 S  
SR CA  
LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



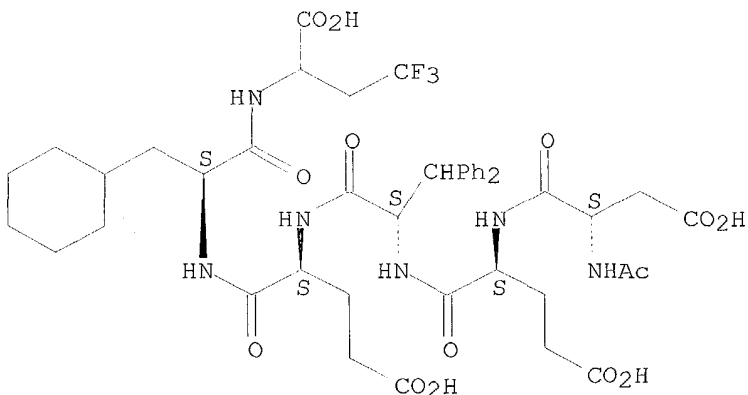
1 REFERENCES IN FILE CA (1907 TO DATE)  
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REFERENCE 1: 132:36034

L5 ANSWER 16 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 252355-91-2 REGISTRY  
CN Butanoic acid, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-L-alanyl-2-amino-4,4,4-trifluoro- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C44 H55 F3 N6 O14  
SR CA  
LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



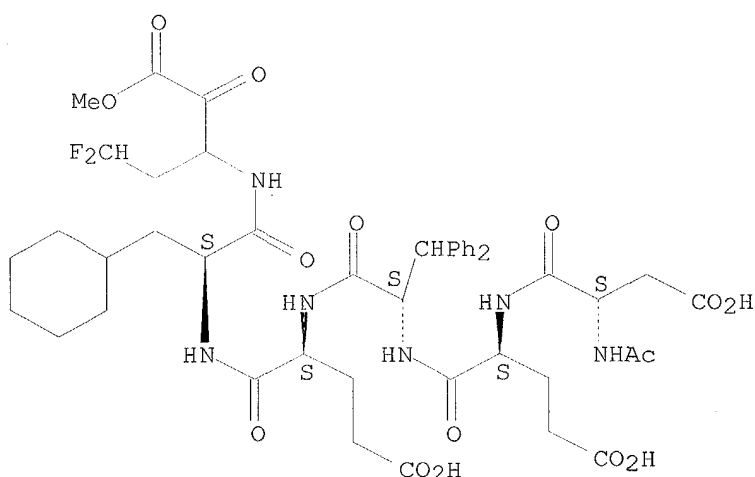
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 17 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 252355-90-1 REGISTRY  
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-  
 phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[1-(2,2-  
 difluoroethyl)-3-methoxy-2,3-dioxopropyl]- (9CI) (CA INDEX NAME)  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C46 H58 F2 N6 O15  
 SR CA  
 LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



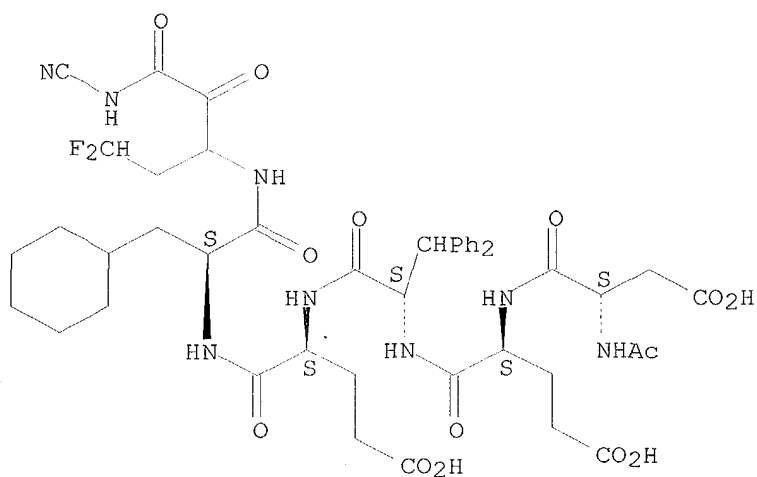
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 18 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 252355-89-8 REGISTRY  
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-  
 phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[3-(cyanoamino)-1-(2,2-  
 difluoroethyl)-2,3-dioxopropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
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 SR CA  
 LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



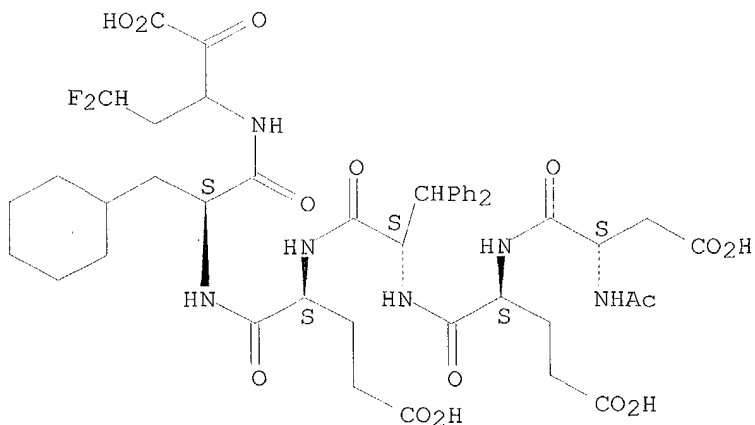
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 19 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 252355-88-7 REGISTRY  
CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-N-[1-(carboxycarbonyl)-3,3-difluoropropyl]-3-cyclohexyl- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C45 H56 F2 N6 O15  
SR CA  
LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



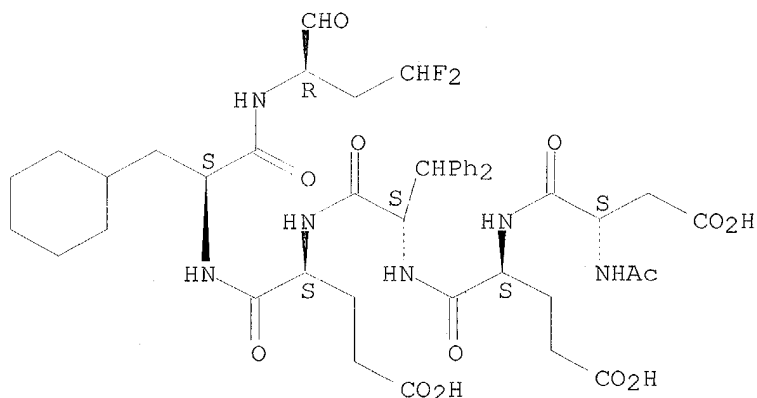
1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 20 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 252355-87-6 REGISTRY  
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[(1R)-3,3-difluoro-1-formylpropyl]- (9CI) (CA INDEX NAME)  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C44 H56 F2 N6 O13  
 SR CA  
 LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



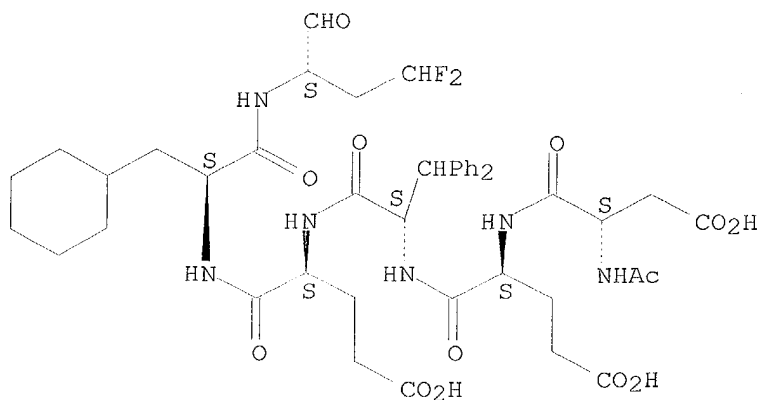
1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:36034

L5 ANSWER 21 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 252355-86-5 REGISTRY  
 CN L-Alaninamide, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-N-[(1S)-3,3-difluoro-1-formylpropyl]- (9CI) (CA INDEX NAME)  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C44 H56 F2 N6 O13  
 SR CA  
 LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

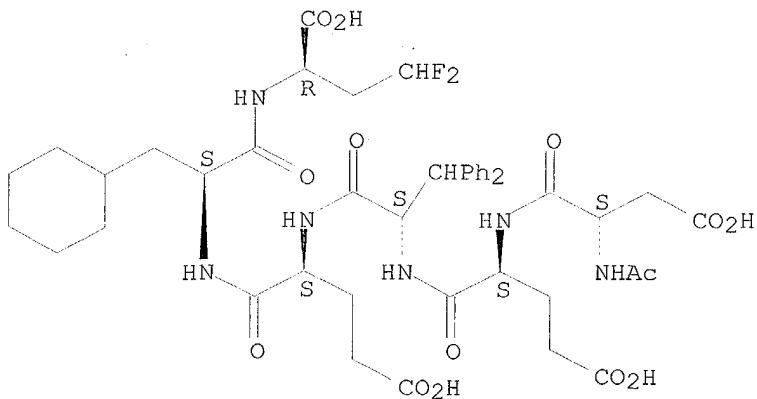
REFERENCE 1: 137:149812

REFERENCE 2: 132:36034

L5 ANSWER 22 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
RN 252355-85-4 REGISTRY  
CN Butanoic acid, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-L-alanyl-2-amino-4,4-difluoro-, (2R)- (9CI) (CA INDEX NAME)  
FS PROTEIN SEQUENCE; STEREOSEARCH  
MF C44 H56 F2 N6 O14  
SR CA  
LC STN Files: CA, CAPLUS

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812

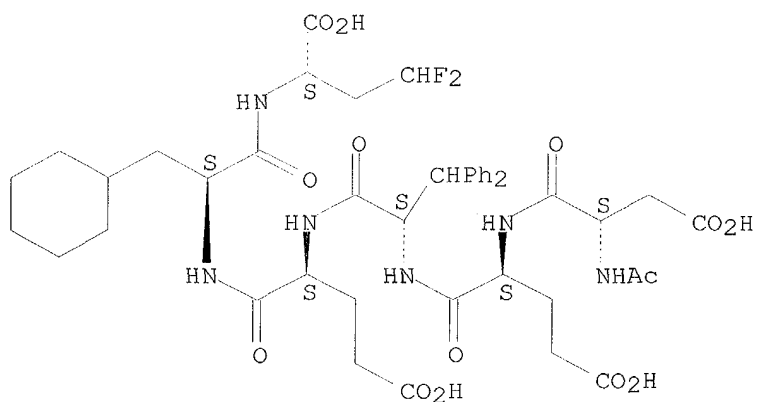
REFERENCE 2: 132:36034



L5 ANSWER 23 OF 23 REGISTRY COPYRIGHT 2003 ACS on STN  
 RN 252355-84-3 REGISTRY  
 CN Butanoic acid, N-acetyl-L-.alpha.-aspartyl-L-.alpha.-glutamyl-.beta.-  
 phenyl-L-phenylalanyl-L-.alpha.-glutamyl-3-cyclohexyl-L-alanyl-2-amino-4,4-  
 difluoro-, (2S)- (9CI) (CA INDEX NAME)  
 FS PROTEIN SEQUENCE; STEREOSEARCH  
 MF C44 H56 F2 N6 O14  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

\*\*RELATED SEQUENCES AVAILABLE WITH SEQLINK\*\*

Absolute stereochemistry.



3 REFERENCES IN FILE CA (1907 TO DATE)  
 3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:149812  
 REFERENCE 2: 132:245829  
 REFERENCE 3: 132:36034